

Software

Unintentional fragment handling

Overview

Unintentional fragmentation, also known as transmission-related fragmentation (which can include adducts, dimers, isotopes, and in-source fragmentation), occurs during the mass spectrometry process, where ions may break apart as they pass through the instrument. These additional ion signals complicate data interpretation and reduce reliability unless handled correctly. Thermo Scientific™ Compound Discoverer™ software 3.4 introduces a new feature-based workflow with advanced transmission-related fragment handling capabilities, automating the identification and reduction of transmission-related fragments to enhance data clarity and accuracy.

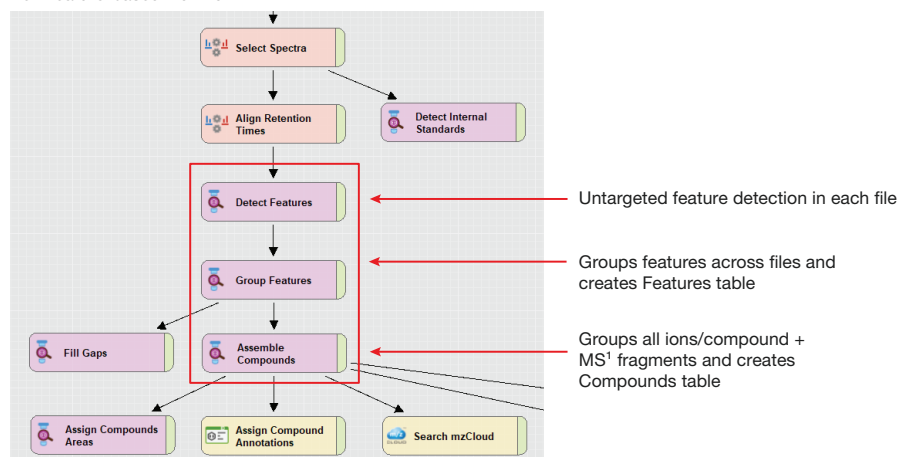
Method

Compound Discoverer software matches transmission-related fragments with the precursor by correlating fragmentation data from the MS² scan with peaks that are detected in the full scan. To increase confidence, Compound Discoverer software also makes use of the low collision energy information that is available from the mzCloud™ spectral library. For compounds that can be matched to the data based on authentic standards in mzCloud, Compound Discoverer software automatically retrieves the scan with the lowest collision energy that is available in the spectral library and uses this information to confirm the association between a suspected transmission-related fragment and the precursor.

Key features

- 1. Automated fragment identification:** The new algorithm in Compound Discoverer software 3.4 automatically identifies transmission-related fragments, which were previously managed manually, and reduces them into a single compound. This feature simplifies your analysis and ensures that data processing is more efficient and less prone to human error.
- 2. Comprehensive data reduction:** The automation of transmission-related fragment handling reduces the need for manual intervention, speeding up the data processing workflow so you can focus on data interpretation and analysis.
- 3. Enhanced data clarity:** By eliminating chemical noise and artifacts, the software provides a clearer and more accurate representation of the actual compounds present in the sample. This leads to more reliable results in your metabolomics research.
- 4. Confident purity assessment:** There is so much stuff in complicated samples, even with best separations and methods you may inevitably have coelutions. The new MS² purity column in the compounds table provides a measurable degree of chimerism within an RT window for each compound, helping you build confidence in the clarity of your data.

New feature-based workflow



New feature-based workflow | Compounds table with Features sub-table

Compounds											
Compounds per File			Features			Internal Standards			Internal Standards per File		
#	Name	Formula	Annot. Source	Annot. ΔMa	Calc. MW	m/z	Reference Ion	RT [min]	Area (Max.)	Polarity	MS2
1	Citric acid	C6 H8 O7		-0.79	192.02685	191.01953	[M-H]-1	2.465	2053592021	+/-	100
2	α-Lactose	C12 H22 O11		-0.14	342.11616	685.23962	[2M+H]+1	1.337	587538199	+/-	100

Structure Proposals											
Compounds per File			Predicted Compositions			Features			LipidSearch Results		
#	Ion	Charge	Adduct Feature	Molecular Weight	m/z	RT [min]	FWHM [min]	Area (Max.)	Intensity (Max.)	# MI (Max)	MS2
1	[M-H]-1	-1	Yes	192.02681	191.01953	2.463	0.072	2053592021	398788672	3	100
2	[2M+Na]+1	1	Yes	192.02699	407.04319	2.464	0.074	177434530	35446957	4	97
3	[M+K]+1	1	Yes	192.02698	230.99014	2.448	0.084	32650816	5585975	3	89
4	[M+NH4]+1	1	Yes	192.02703	210.06085	2.465	0.079	21019256	3808026	3	100
5	[2M+H]+1	1	Yes	192.02703	385.05541	2.464	0.057	8827391	2363702	2	100
6	[2M-H]-1	-1	Yes	192.02703	385.05541	2.453	0.064	6669654	1686510	2	100
7	[M+Na]+1	1	Yes	192.02698	193.03421	2.481	0.088	301799906	45281828	3	100
8	[M+H]+1	1	Yes	192.02694	193.03421	2.463	0.066	91676624	19324864	3	100
9	[X-e]+1	1	No	147.02936	147.02881	2.460	0.065	109530488	24271686	3	99
10	[X-e]+1	1	No	147.02936	147.02881	2.460	0.065	83755928	18422246	3	99
11	[X-e]+1	1	No	147.02936	147.02881	2.460	0.065	45920575	9881318	2	99
12	[X-e]+1	1	No	147.02936	147.02881	2.460	0.065	11645776	2637905	2	98

New columns in the Compounds table

Compounds											
Compounds per File			Features			Internal Standards			Internal Standards per File		
#	Comments	Name	Formula	Annot. Source	Annot. ΔMa	Calc. MW	m/z	Reference Ion	RT [min]	Area (Max.)	Polarity
1	check	Citric acid	C6 H8 O7		-0.79	192.02685	191.01953	[M-H]-1	2.465	2053592021	+/-
2		α-Lactose	C12 H22 O11		-0.14	342.11616	685.23962	[2M+H]+1	1.337	587538199	+/-
3	interesting!	3-Methyl-1,3-benzothiazol-5-ylidene-L-proline	C9 H8 N2 S		1.10	180.06336	113.03462	[M+H+2O]+	14.532	413373613	+
4		D-Glucose	C6 H12 O6		-0.16	180.06336	113.03462	[M+CB]-1	1.280	405793436	-
5		Acetyl-L-carnitine	C9 H17 N O4		-1.57	203.11544	204.12272	[M+H]+1	2.027	310159287	+
6		αa-Trehalose	C12 H22 O11		-0.24	342.11613	387.11412	[M+FA-H]-1	1.552	258027598	+/-
7		Creatine	C4 H9 N3 O2		-0.18	131.06945	132.07673	[M+H]+1	1.395	236191312	+
8		C28 H47 Cl O15 P2			1.31	720.20882	719.20154	[M-H]-1	1.311	210960127	-
9		Choline Alfoscerate	C8 H20 N O6 P		0.38	257.10292	258.11020	[M+H]+1	1.291	203089800	+
10		Lauryldiethanolamine	C16 H35 N O2		-0.14	273.26674	274.27402	[M+H]+1	10.406	181739678	+
11			C2 H5 N3 O3 P2		-3.64	180.97995	163.97668	[M+H+2O]+	14.883	172451570	+
12		trans-Aconitic acid	C6 H6 O6		-0.23	174.01640	175.02367	[M+H]+1	2.461	158686720	+/-

$$\text{MS}^2 \text{ Purity} = \frac{\text{intensity of target mass centroid}}{\text{total intensity of all centroids within isolation window}} \times 100$$

Benefits

- Efficiency:** Automated processes save time and reduce the workload on researchers.
- Accuracy:** Improved fragment handling ensures more precise identification of compounds.
- Data quality:** Reduction of chemical noise and artifacts leads to higher quality data and more reliable results.

Conclusion

The transmission-related fragment handling capabilities in Compound Discoverer software 3.4 streamline the data processing workflow, providing researchers with a powerful tool to achieve more accurate and efficient metabolomics analysis.

Learn more at thermofisher.com/compounddiscoverer